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Integrated computational material engineering model development for tube drawing process

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Abstract

In order to be able to understand the tube drawing process in a better way and also to analyze more complex situations, multiscale simulation approach based on the Integrated Computational Materials Engineering was used and an FEM model was developed. The responsibility of this model was to get the eccentricity and residual stresses of the tubes before the drawing process and simulate the same parameters and their variations during the drawing. For simulation, the multiscale methodology based on the idea of Integrated Computational Materials Engineering was used to study the process. The main reason for using the multiscale simulation methodology was to study plastic behavior of the material in the FEM model considering texture of the material.

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Keywords: Multiscale simulation; Tube drawing; Crystal plasticity; Integrated computational materials engineering; FEM.

1. Introduction

Tubes have a very wide range of applications, so being used in automotive and aerospace industries, medical services, plumbing as well as structural elements in buildings or bridges. Long lasting copper tubes are a favorite choice for plumbing, heating, cooling and other systems [1]. Generally speaking, tubes can be without seam or with seam. Tubes without seam (seamless tubes) are produced mostly by extrusion and piercing methods. The tubes with

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seam, however, are produced by the various welding techniques [2]. Each of these methods has their specific advantages and disadvantages. Furthermore, depending on the application requirements, tubes are manufactured in different sizes and shapes. Due to the ever-increasing competition with the advent of globalization it has become highly important to keep on improving the process efficiency in terms of product quality, precision, and optimized use of resources. The factors that determine the choice of the forming or for that matter any other process are maximum utilization of resources with high quality output [3]. In cold drawing process, like any other forming processes, drawn tubes have also some imperfections, which influence their quality and performances. It is critical to understand the relationships between the individual steps in production of tubes; casting, extrusion, and cold drawing, and connect them into one continuous process

The seamless tube-making process often causes wall-thickness variations which on one hand increase the weight of the final products and on the other hand causes some unnecessary costs for the plant. To obtain a minimum wall thickness in a tube, which has differences in wall thickness, more metal is needed to get the pre-set minimum wall thickness. On the other hand, the thinnest part of the tube is the main part which the strength of the tube is measured and therefore having a huge difference in wall thickness cause an extra material to produce a tube with pre-set strength. Thus, the material cost of such a tube having a variable wall thickness exceeds that of a tube having a uniform wall thickness. For this reason, optimizing the standard tube drawing process to control the eccentricity of the tubes during drawing in a reproducible way was necessary [4].

In this work in order to be able to understand the tube drawing process in a better way and also to analyze more complex situations, multiscale simulation approach based on the ICME was used and an FEM model was developed. The responsibility of this model was to get the eccentricity, RSs of the tubes before the drawing process and simulate the same parameters and their variations during the drawing. In the ICME methodology, the material models as well as structure – property relationships are integrated, which these properties are observed from experiments and simulations [5]. The advantages of ICME approach include the following:

- Reduce product development time; ICME eases the costly trial and error physical design iterations (design cycles) and facilitate far more cost-effective virtual design optimization.
- Reduce product costs by creating new material, product, and also process designs.
- Increase product quality and performance by providing more accurate predictions of response to design loads.

Nomenclature

ICME	Integrated Computational Material Engineering
DFT	Density Function Theory
GSFE	Generalized Stacking Fault Energy
MEAM	Modified Embedded-Atom Method
MD	Molecular Dynamics
DD	Dislocation Dynamics
CP	Crystal Plasticity
FEM	Finite Element Method
RSs	Residual Stresses

2. Model development

A multiscale simulation model based on the idea of ICME to study the tube drawing process was developed. This methodology starts with the electronic scale calculations, which is done by DFT approach by the Quantum Espresso software. The most important parameter in this simulation length was the calculation of energy variation as a function of lattice parameter (E-A diagram). After achieving the required data, these data were bridged to the next simulation scale, which was the atomic scale calculation, using MD, in which the dislocation velocity as calculated. In next step DD approach was used and hardening parameters in Palm-Voce hardening equation were computed. These parameters were used in CP simulations to be imported in the FEM model, which was created for the tube drawing process. Eccentricity and RSs of the tubes were measured and imported to the FEM model. The simulation results were validated using the simulated and measured eccentricities, RSs, and mechanical properties (stress-strain diagram). The multiscale methodology is shown in Fig. 1 schematically, which was used to achieve all the necessary parameters for the final FEM simulations.

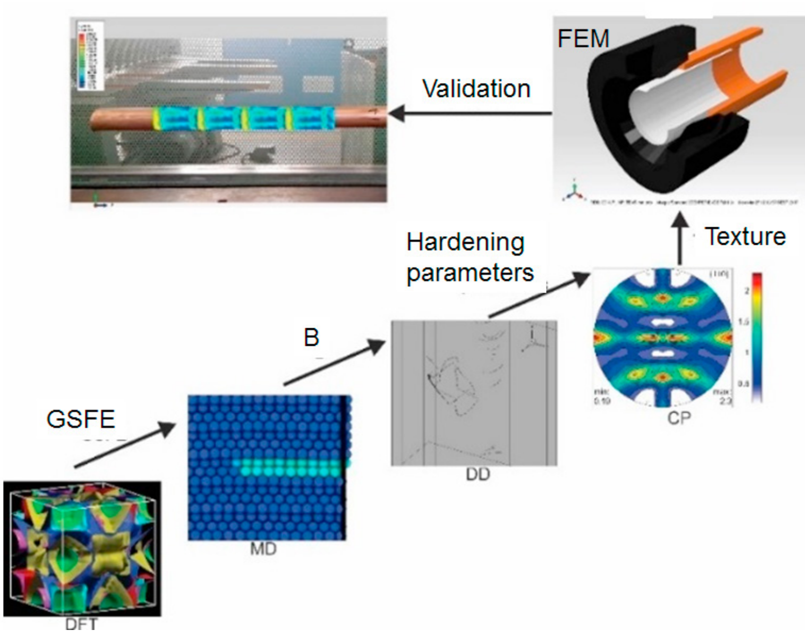

Fig. 1. Schematic showing the bridges for upscaling related to garnering the plasticity information for forming finite element simulations.

The bridges, which were used in this work and as illustrated in the above figure, are explained briefly in the following:

Bridge 1: Using DFT calculations, the lattice parameter, bulk modulus, energy variation and GSFE were calculated for copper. These parameters were upscaled for the 2nd bridge.

Bridge 2: Calculating the dislocation mobility by MD.

Bridge 3: Calculating the hardening parameters and drag coefficient from DD calculations with the dislocation mobility, which was calculated in the previous bridge.

Bridge 4: Using CP method, the texture of material was imported to the FEM model and the hardening parameters were used here for FEM calculations.

For FEM simulation, Abaqus 2016 was used [6]. To incorporate the CP into the FEM, UMAT user subroutine – UMAT is a user subroutine to define a material's mechanical behavior [7] – was used and with this subroutine it was possible to insert the anisotropic elastic constants (calculated by MEAM), hardening parameters (calculated by DD), and measured texture (Euler angles) into the FEM simulations.

3. Results and discussion

The electronic scale simulation was done using DFT approach by Quantum Espresso software. The main parameters, calculated in this simulation scale, were: The lattice parameter, the energy of crystal lattice by variation of the lattice parameter, bulk modulus, and most importantly GSFE. The setup, which has been chosen for the simulation, was an *fcc* structure with an initial guess for lattice parameter of copper, which was 6.824 Bohr or 3.61 Å. This initial guess was necessary to start the calculations. The method used for occupation was the electron smearing method. This technique allows for electrons to have a fractional occupation number by creating an energy window [302]. All used parameters are shown in Table 1.

Table 1. Parameter used in the electronic scale simulation as input.

Parameter	Value	Source
Crystal structure	fcc	-
Cell dimension	6.824 bohr / 3.61 Å	[8]
E_{cut}	30 Ry / 408 eV	[8]
Occupation	Smearing	[9]
Atomic weight	63.54 g/mol	[8]
Psudopotential	Cu.pbesol-dn-kjpaw_psl.0.2.UPF	[10]
K-point	2 - 20	-
Cohesive energy	3.49 eV/atom	[11]

The variations of the energy as a function of the lattice parameter were calculated using DFT simulation technique. Fig. 2 shows the variation of the energy of fcc crystal structure of copper by variation of the lattice parameter. As can be seen, the minimum energy is achieved for the lattice parameter of the copper, which explains why copper atoms like to have this lattice parameter.

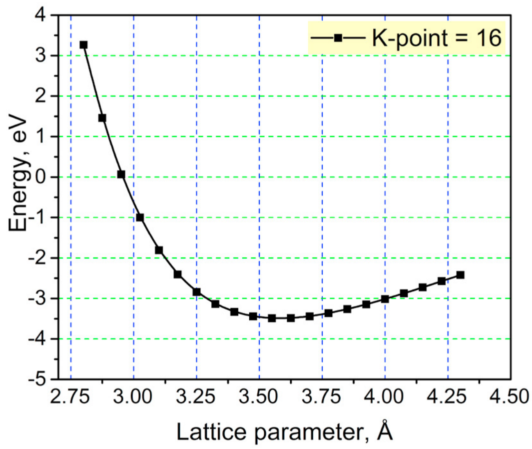

Fig. 2. Energy changes by changing the lattice parameter of copper.

To calculate the dislocation velocity a simulation box in LAMMPS solver (regarding MD calculations) was created and different shear stresses were applied on this simulation box. The applied shear stresses made the edge dislocation (Burgers vector of $[\bar{1}01]$) to glide and created a step between upper and lower side of the simulation box, which is shown in Fig. 3(a). For each applied shear stress, the displacement of the dislocation was measured as a function of time. This matter is shown in Fig. 3(b). Using these results the dislocation velocity at each applied shear stress was calculated.

After calculating the dislocation velocity by MD, Palm-Voce hardening Eq. (1) was used and the hardening parameters (κ_s , h_0, and κ_0) were calculated using DD simulations, which were 148, 180 and 16 MPa, respectively. Variation of κ with the plastic strain is presented in Fig. 4.

$$\kappa = \kappa_s - (\kappa_s - \kappa_0)\, exp\left(-\frac{h_0}{\kappa_s - \kappa_0} Ct\right). \quad (1)$$

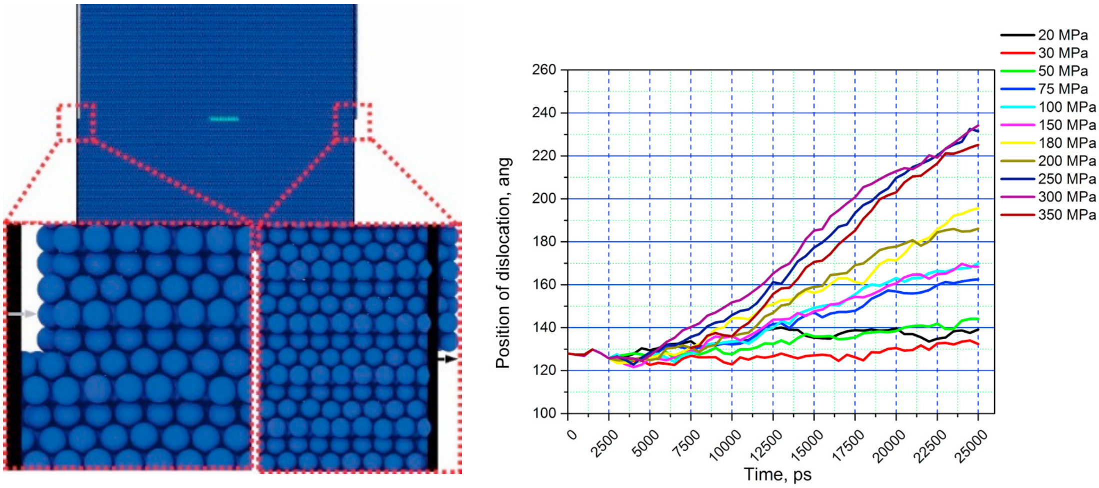

Fig. 3. (a) Creation of step due to movement of simulation box, which is because of the applied shear stress; (b) position of dislocation as function of time.

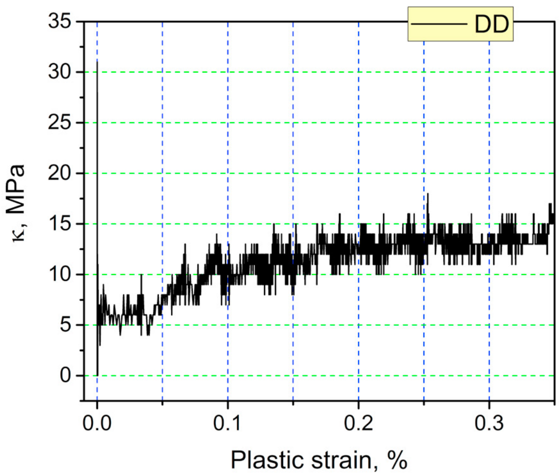

Fig. 4. Variation of κ by changing of the plastic strain.

Different tubes with different measured-eccentricity were created for the FEM simulations in Solidworks software. The used die and plug were created with real dimensions in the FEM software (Abaqus) and were considered as rigid bodies. The measured RSs with neutron diffraction were also imported into the software using a Sigini subroutine. The assembly of the developed FEM model is shown in Fig. 5. Table 2 summarizes all the parameters and inputs used in FEM simulations.

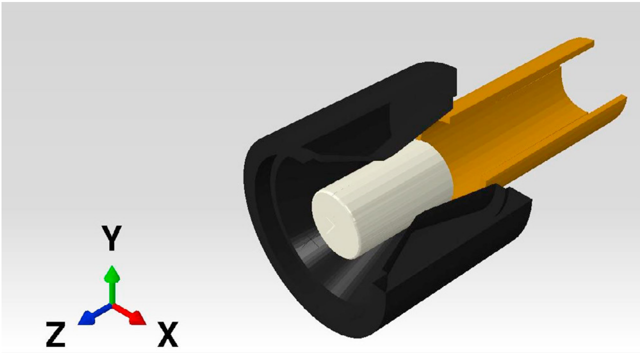

Fig. 5. Assembly of 1st drawing step, showing tube, die and plug.

Table 2. Different parameters used in FEM simulations.

Input	Tubes' diameter	Experimentally measured
Tube Properties	Tubes' eccentricity	Experimentally measured
	Tubes' RSs	Experimentally measured
	Tubes' texture	Experimentally measured
	Elastic parameters	Calculated atomic scale
	Plastic parameters	Calculated microscale
	Parameters of slipping rate	Literature
Die and plug	Dimensions	Exp. Measured
	Behavior	Rigid body
Step	Dynamic, implicit	
Interaction	Penalty	
Friction coefficient	0.05	
Element type	C3DR8	
Drawing velocity	0.33 m/s – 20 m/min	

The simulated RSs in axial, hoop, and radial directions at Max of the drawn tube are shown in Fig. 6(a). To compare these results with the measured RSs at the same tube and same positions, the measured RSs are shown in the same diagrams, as well [12]. The solid and dashed lines depict the experimentally measured and simulated RSs, respectively. As can be clearly seen, the results in all 3 directions and positions are close to each other, showing that the model is valid respect to the RSs.

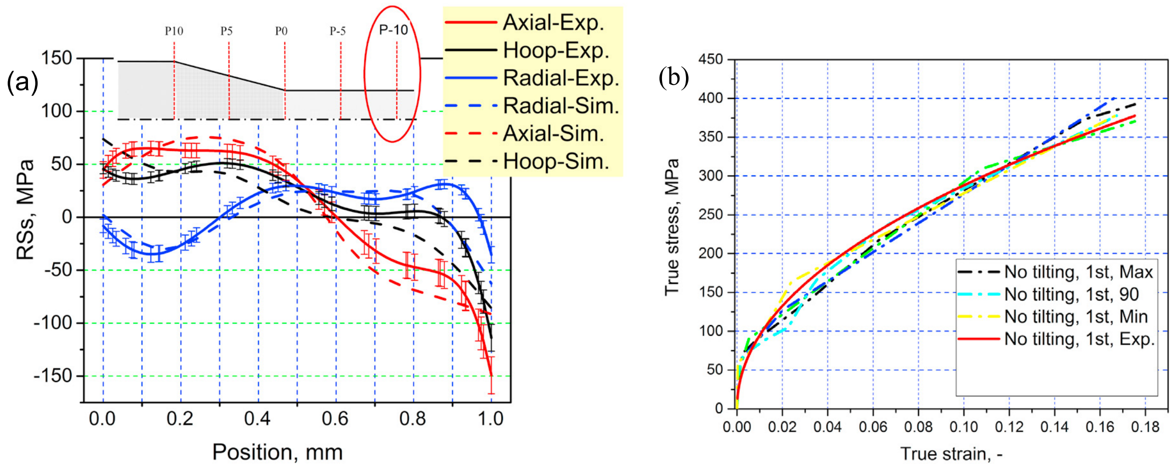

Fig. 6. (a) Simulated and measured (by neutron diffraction method [12]) RSs in axial, hoop, and radial directions in the drawn tube; (b) simulated and measured stress-strain diagrams of drawn tube.

4. Conclusion

In order to study eccentricity and RSs in tube drawing process, multiscale simulation method using ICME approach was used. Anisotropic behavior of the copper tubes was simulated by considering anisotropic elastic and plastic parameters. On the other hand, since tube drawing is a process with a quite high deformation, the behavior of the dislocation and the hardening of the material is an important factor in the simulation of such process. To consider all these parameters in the simulations, different length scale simulations were performed.

By electronic scale simulation, DFT was used and the energy variation of an fcc structure as a function of lattice parameter was calculated. In next step a simulation box in MD simulations was created and different shear stresses were applied to this simulation box and the movement of the dislocation was calculated and subsequently, the dislocation velocity was calculated at each applied shear stress. The dislocation mobility was bridged to the next simulation scale, which was the microscale simulation using DD method. At this level, a simulation box with a specific dislocation density was created and this box was deformed with a specific strain rate and the achieved mechanical properties were used to get the hardening parameters of the hardening equation, which was the Palm-Voce hardening. These parameters were bridged to upper simulation level. Mesoscale simulations were done using CP method and a UMAT subroutine was used to implement this method into the FEM simulations. A model for tube drawing with and without tilting angle was created in the Abaqus FEM software package.

Acknowledgements

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References

[1] M. Hashmi, Aspects of tube and pipe manufacturing processes: Meter to nanometer diameter, 3rd Brazilian Congress on Manufacturing Engineering, 179-1-3 (2006) 5–10.
[2] P.C. Sharma, Mecahnical working of metals, In A Textbook of Production Technology: Manufacturing processes, P.C. Sharma, Ed., INDIA: S. Chand Publishing, (2009) 212–321.
[3] B. Kumar, A. Singh, S. Das, D. Bhattacharya, Cold rolling texture in AISI 304 stainless steel, Materials Science and Engineering: A, 364-1-2 (2004) 132–139.
[4] F. Foadian, A. Carradó, H. Palkowski, Precision tube production: Influencing the eccentricity and residual stresses by tilting and shifting, Journal of Materials Processing Technology, 222 (2015) 155–162.
[5] F. Horstemeyer, Integrated computational materials engineering (ICME) for metals: Using multiscale modeling to invigorate engineering design with science, Hoboken, N.J.: (2012), WILEY-TMS.
[6] R. Abbaschian, R.E.R. Hill, L. Abbaschian, Physical metallurgy principles, 4th edition, Stamford, Conn.: Cengage Learning, (2009).
[7] Hibbitt, Abaqus 2016 Documentation, USA: Hibbitt, Karlsson, and Sorensen, Inc, (2016).
[8] E.S. Drexler, N.J. Simon, R.P. Reed, Properties of copper and copper alloys at cryogenic temperatures, NIST NIST-MN-177, (1996).
[9] M.C. Michelini, R.P. Diez, A.H. Jubert, A density functional study of small nickel clusters, International Journal of Quantum Chemistry, 70-4-5 (1998) 693–701.
[10] Quantum Espresso, Pseudopotentials. Available: http://www.quantum-espresso.org/pseudopotentials/
[11] Copper, The Periodic Table at Knowledge Door.
[12] F. Foadian, A. Carradó, T. Pirling, H. Palkowski, Residual stresses evolution in Cu tubes, cold drawn with tilted dies – Neutron diffraction measurements and finite element simulation, Materials & Design, 107 (2016) 163–170.